MATH337: Changepoint Detection

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Table of contents

Pr	eface		4
	Sour	rce files, and attributions	5
1	An l	Introduction to Changepoint Detection	6
	1.1	Piecewise Stationary Time Series	6
		1.1.1 What is a time series?	6
		1.1.2 Stationary, non-stationary, and piecewise stationary time series	8
	1.2	Introduction to changepoints	10
		1.2.1 Types of Changes in Time Series	13
		1.2.2 The biggest data challenge in changepoint detection	15
	1.3	Detecting one change in mean	16
		1.3.1 The CUSUM statistics	17
		1.3.2 Algorithmic Formulation of the CUSUM Statistic	18
		1.3.3 Example	20
	1.4	Exercises	21
		1.4.1 Workshop 1	21
		1.4.2 Lab 1	22
2	Con	strolling the CUSUM and Other Models	23
	2.1	The asymptotic distribution of the CUSUM statistics	23
		2.1.1 Controlling the max of our cusums	24
	2.2	The Likelihood Ratio Test	26
		2.2.1 Example: Gaussian change-in-mean	27
	2.3	Towards More General Models	28
		2.3.1 Change-in-variance	28
		2.3.2 Change-in-slope	29
		2.3.3 Revisiting our Simpsons data (again!)	31
	2.4	Exercises	33
		2.4.1 Workshop 2	33
		2.4.2 Lab 2	33
3	Mul	Itiple changepoints	35
	3.1	Introduction	35
		3.1.1 Real Example: Genomic Data and Neuroblastoma	35
		3.1.2 Towards multiple changes	36

		3.1.3 The cost of a segmentation	38
		3.1.4 The "best" segmentation	39
	3.2	Binary Segmentation	42
		3.2.1 Binary Segmentation in action	43
	3.3	Optimal Partitioning	48
		3.3.1 Optimal partitinioning in action	49
		3.3.2 Neuroblastoma example	52
	3.4	Exercises	53
		3.4.1 Workshop 3	53
		3.4.2 Lab 3	54
4	PEL	T, WBS and Penalty choices	55
	4.1	Drawbacks of OP and BS	55
		4.1.1 Quality of the Segmentation	55
		4.1.2 Computational Complexity	57
	4.2	PELT and WBS	58
		4.2.1 PELT: an efficient solution to OP	58
		4.2.2 WBS: Improving on Binary Segmentation	60
	4.3	Penalty Selection	61
		4.3.1 Example in R: Comparing Penalties with PELT	62
		4.3.2 CROPS: running with multiple penalties	64
	4.4	Exercises	66
		4.4.1 Workshop 4	66
		4.4.2 Lab 4	67
Re	eferen	nces	69

Preface

These are the notes for MATH337 Changepoint Detection. They were written by Gaetano Romano.

The module will introduce you to changepoint detection, detailing some algorithms, developing the basics theoretical foundations, and practicing few real-world scenarios.

Across five weeks we will cover the following topics:

- 1. An introduction to changepoint detection and the CUSUM statistics
- 2. Controlling the CUSUM and some additional models
- 3. Dealing with multiple changes
- 4. PELT, WBS and Penalty selection
- 5. Working with Real World data.

We will be using R as the programming language for this module. If you're unfamiliar with it, make sure you cover the first three weeks of MATH245.

Every week, you are expected to follow two lectures, one workshop, and one computer aided lab. Over the lecture, we will cover the basics concepts of changepoint detection.

At the end of each chapter, you will find exercises that will be carried in the workshop and the lab. During the workshop, you will be dealing with computations and details about the methodologies introduced at your own pace, and, finally, during the workshops, you'll give a go at programming the various algorithms and running real-world examples.

You will find the solutions to the exercises on the Moodle page, released weekly. If you cannot access the Moodle page, and you still would like to have these solutions, please get in touch with me.

Source files, and attributions

The notes are released as open-source on GitHub under the CC BY-NC 4.0 License. You can access the repository at the following link: https://github.com/gtromano/MATH337_change point_detection.

The materials in this course are based on and share elements with the following resources:

- Fearnhead, P., & Fryzlewicz, P. (2022). Detecting a single change-point. arXiv preprint arXiv:2210.07066.
- Rebecca Killick's Introduction to Changepoint Detection a half-day introductory course on changepoint detection.
- Rebecca Killick's Further Changepoint Topics an extended course on changepoint detection.
- Toby Hocking's Course on Unsupervised Learning, which includes changepoint detection.

I would like to express my gratitude to the authors of these resources. In addition, materials were sourced from various academic papers, which are referenced throughout the body of these notes.

1 An Introduction to Changepoint Detection

1.1 Piecewise Stationary Time Series

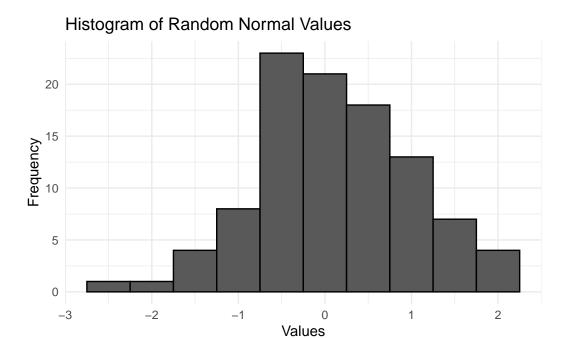
In this module, we will be dealing with **time series**. A time series is a sequence of observations recorded over time (or space), where the order of the data points is crucial.

1.1.1 What is a time series?

In previous modules, such as Likelihood Inference, we typically dealt with data that was not ordered in a particular way. For example, we might have worked with a sample of independent Gaussian observations, where each observation is drawn randomly from the same distribution. This sample might look like the following:

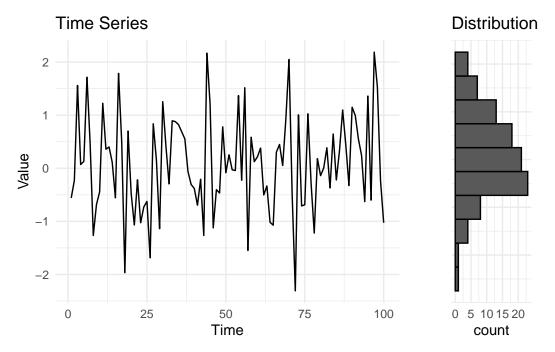
$$y_i \sim \mathcal{N}(0, 1), \ i = 1, \dots, 100$$

Here, y_i represents the *i*-th observation, and the assumption is that all observations are independent and identically distributed (i.i.d.) with a mean of 0 and variance of 1.



In this case, the observations do not have any particular order, and our primary interest may be in estimating parameters such as the mean, variance, or mode of the distribution. This is typical for traditional inference, where the order of observations is not of concern.

However, a **time series** involves a specific order to the data—usually indexed by time, although it could also be by space or another sequential dimension. For example, we could assume that the Gaussian sample above is a sequential process, ordered by the time we drew an observation. Each observation corresponds to a specific time point t:



Formal Notation. In time series analysis, we typically denote a time series by using an index t to represent time or order. The time series vector is written as:

$$y_{1:n}=(y_1,y_2,\dots,y_n)$$

Here, n is the total length of the sequence, and y_t represents the observed value at time t, for t = 1, 2, ..., n. In our previous example, for instance, n = 100.

Often, we are also interested in subsets of a time series (inclusive), especially when investigating specific "windows" or "chunks" of the data. We will denote as a subset of the time series, from time l to time u, the following:

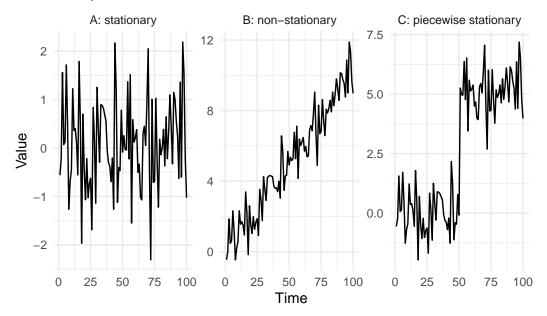
$$y_{l:u} = (y_l, y_{l+1}, \dots, y_u)$$

Understanding and working with subsets of time series data is important for many applications, such as when detecting changes in the behavior or properties of the time series over specific intervals.

1.1.2 Stationary, non-stationary, and piecewise stationary time series

Time series can be classified into different categories based on their statistical properties over time. The three main types are **stationary**, **non-stationary**, and **piecewise stationary** time series. For example:

Comparison of Time Series



1. **Stationary Time Series**: A time series is said to be *stationary* if its statistical properties—such as the mean, variance, and autocovariance—are constant over time. This implies that the behavior of the series doesn't change as time progresses.

Mathematically, for a stationary time series y_t , the expected value and variance are constant over time:

$$\mathbb{E}(y_t) = \mu \quad \text{and} \quad \text{Var}(y_t) = \sigma^2 \quad \forall \in \{1,...,n\}$$

In this example, the stationary time series was generated by sampling random normal variables $y_t = \epsilon_t$, $\epsilon_t \sim \mathcal{N}(0, 1)$. We can see, very simply how, in this case:

$$\mathbb{E}(y_t) = \mathbb{E}(\epsilon_t) = 0, \forall t \in \{1, ..., 100\}$$

2. **Non-Stationary Time Series**: A time series is *non-stationary* if its statistical properties change over time. Often, non-stationary series exhibit trends or varying variances. For example, a series with a trend (increasing or decreasing) is non-stationary because the mean is not constant.

A common form of non-stationarity is a linear trend, where the series grows over time. In our example, the non-stationary series is generated as:

$$y_t = \epsilon_t + 0.1 \cdot t, \ \epsilon_t \sim \mathcal{N}(0, 1)$$

This creates a time series with a linear upward trend. In fact, similarly to what done before:

$$\mathbb{E}(y_t) = \mathbb{E}(\epsilon_t) + \mathbb{E}(0.1 \cdot t) = 0.1 \cdot t.$$

Therefore:

$$\forall t_1, t_2 \in \{1, ..., 100\}, t_1 \neq t_2 \rightarrow \mathbb{E}(y_{t_1}) \neq \mathbb{E}(y_{t_2})$$

3. **Piecewise Stationary Time Series**: A *piecewise stationary* time series is stationary within certain segments but has changes in its statistical properties at certain points, known as *changepoints*. After each changepoint, the series may have a different mean, variance, or both.

In our example, the time series was stationary for the first half of the observations, but after t = 50, a sudden shift occurs. Mathematically:

$$y_t = \begin{cases} \epsilon_t & \text{for } t \leq 50 \\ \epsilon_t + 5 & \text{for } t > 50 \end{cases}, \quad \epsilon_t \sim \mathcal{N}(0, 1)$$

This abrupt change at t = 50 introduces a piecewise structure to the data.

1.2 Introduction to changepoints

Changepoints are sudden, and often unexpected, shifts in the behavior of a process. They are also known as breakpoints, structural breaks, or regime switches. The detection of changepoints is crucial in understanding and responding to changes in various types of time series data.

The primary objectives in detecting changepoints include:

- Has a change occurred?: Identifying if there is a shift in the data.
- If yes, where is the change?: Locating the precise point where the change happened.
- What is the difference between the pre and post-change data? This may reveal the type of change, and it could indicate differences in parameter values before and after the change.
- How certain are we of the changepoint location?: Assessing the confidence in the detected changepoint.
- How many changes have occurred?: Identifying multiple changepoints and analyzing each one for similar characteristics.

Changepoints can be found in a wide range of time series, not limited to physical, biological, industrial, or financial processes, and which objectives to follow depends on the type of the analysis we are carrying.

In changepoint detection, there are two main approaches: **online** and **offline** analysis. In applications that require **online analysis**, the data is processed as it arrives, or in small batches. The primary goal of online changepoint detection is to identify changes as quickly as possible, making it crucial in contexts such as process control or intrusion detection, where immediate action is necessary.

On the other hand, **offline analysis** processes all the data at once, typically after it has been fully collected. The aim here is to provide an accurate detection of changepoints, rather than

a rapid one. This approach is common in fields like genome analysis or audiology, where the focus is on understanding the structure of the data post-collection.

For instance, to give few examples:

1. **ECG**: Detecting changes or abnormalities in electrocardiogram (ECG) data can help in diagnosing heart conditions.

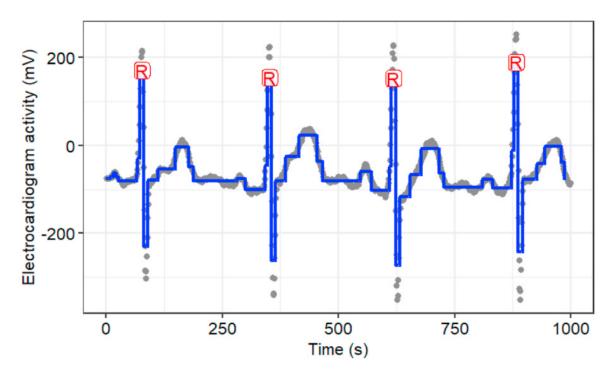


Figure 1.1: Electrocardiograms (heart monitoring), Fotoohinasab et al, Asilomar conference 2020.

2. Cancer Diagnosis: Identifying breakpoints in DNA copy number data is important for diagnosing some types of cancer, such as neuroblastoma. This is a typical example of an offline analysis.

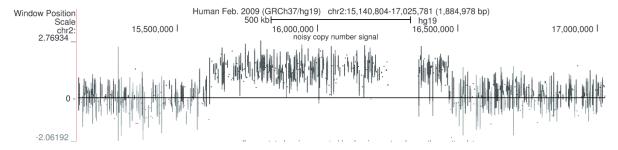


Figure 1.2: DNA copy number data, breakpoints associated with aggressive cancer, Hocking et al, Bioinformatics 2014.

3. **Engineering Monitoring**: Detecting changes in CPU monitoring data in servers can help in identifying potential issues or failures: this is often analysed in real-time on with online methods, with the aim of detecting an issue as quickly as possible.

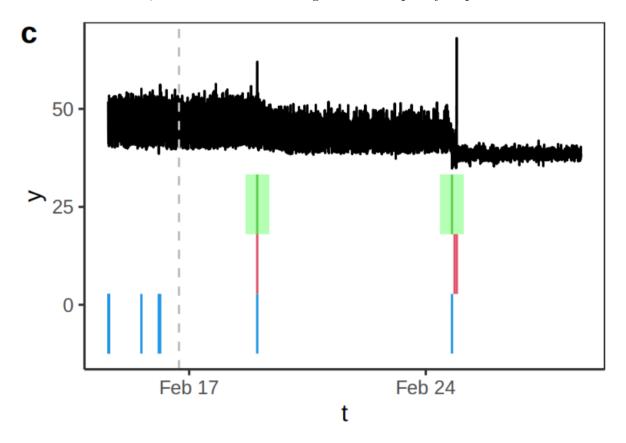


Figure 1.3: Temperature data from a CPU of an AWS server. Source Romano et al., (2023)

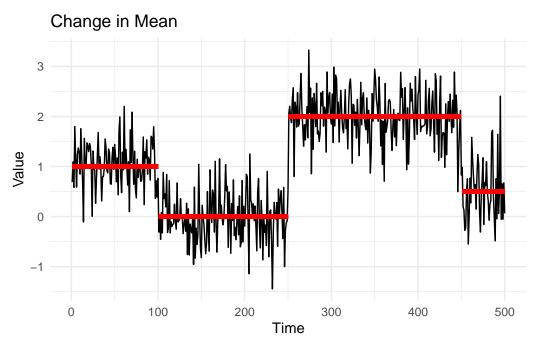
In this module, we will focus exclusively on offline changepoint detection, where we assume

that all the data is available for analysis from the start.

1.2.1 Types of Changes in Time Series

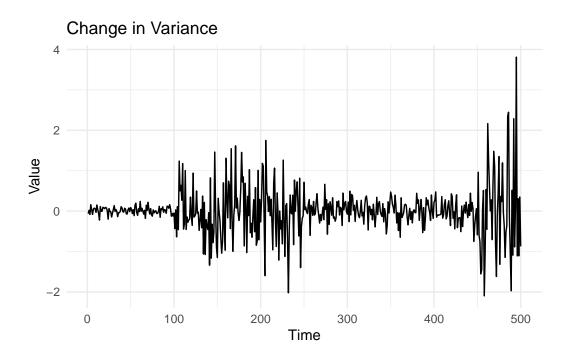
As you might have noticed from the examples above, there's not a strict way on which a timeseries might change. Depending on the model, we could seek for different types of changes in the structure of a time series. Some of the most common types of changes include shifts in mean, variance, and trends in regression. For example, the CPU example above exihibited, in addition to some extreme observations, both changes in mean and variance.

• A **change in mean** occurs when the average level of an otherwise stationary time series shifts from one point to another. This type of change is often encountered in real-world data when there is a sudden shift in the process generating the data, such as a change in policy, market conditions, or external factors affecting the system.



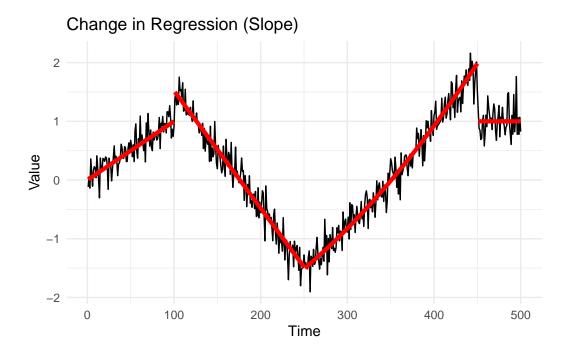
In the plot above, the red lines indicate the true mean values of the different segments.

• A change in variance refers to a shift in the variability of the time series data, even when the mean remains constant. This type of change is important in scenarios where the stability of a process fluctuates over time. For example, in financial markets, periods of high volatility (high variance) may be followed by periods of relative calm (low variance).



1.2.1.1 3. Change in Regression (Slope)

A **change in regression** or slope occurs when the underlying relationship between time and the values of the time series changes. This could reflect a shift in the growth or decline rate of a process. For example, a company's revenue might grow steadily over a period, then plateau, and later exhibit a quadratic or nonlinear growth trend.



1.2.2 The biggest data challenge in changepoint detection

One of the most widely debated and difficult data challenges in changepoint detection may not be in the field of finance, genetics, or climate science—but rather in television history. Specifically, the question that has plagued critics and fans alike for years is: **At which episode did "The Simpsons" start to decline?**

It's almost common knowledge that "The Simpsons," the longest-running and most beloved animated sitcom, experienced a significant drop in quality over time. But pinpointing exactly when this drop occurred is the real challenge. Fortunately, there's a branch of statistics that was practically built to answer questions like these!

I have downloaded a dataset (Bown 2023) containing ratings for every episode of "The Simpsons" up to season 34. We will analyze this data to determine if and when a significant shift occurred in the ratings, which might reflect the decline in quality that so many have observed.



In this plot, each episode of "The Simpsons" is represented by its TMBD rating, and episodes are colored by season. By visually inspecting the graph, we may already start to see some potential points where the ratings decline. However, the goal of our changepoint analysis is to move beyond visual inspection and rigorously detect the exact moment where a significant shift in the data occurs.

Jokes apart, this is a challenging time series! First of all, there's not a clear single change, but rather an increase, followed by a decline. After which, the sequence seems rather stationary. For this reason, throughout the module, we will use this data as a running example to develop our understanding of various methods, hopefully trying to obtain a definitive answer towards the final chapters. But let's proceed with order...

1.3 Detecting one change in mean

In this section, we will start by exploring the simplest case of a changepoint detection problem: **detecting a change in the mean** of a time series. We assume that the data is generated according to the following model:

$$y_t = \mu_t + \epsilon_t, \quad t = 1, \dots, n,$$

where $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$ represents Gaussian noise with mean 0 and known variance σ^2 , and $\mu_t \in \mathbb{R}$ is the signal at time t. The vector of noise terms $\epsilon_{1:n}$ is often referred to as Gaussian noise,

and hence, this model is known as the signal plus noise model, where the signal is given by $\mu_{1:n}$ and the noise by $\epsilon_{1:n}$.

In the change-in-mean problem, our goal is to determine whether the signal remains constant throughout the entire sequence, or if there exists a point τ), where the mean shifts. In other words, we are testing whether:

$$\mu_1 = \mu_2 = \dots = \mu_n$$
 (no changepoint),

or if there exists a time τ such that:

$$\mu_1 = \mu_2 = \dots = \mu_{\tau} \neq \mu_{\tau+1} = \dots = \mu_n$$
 (changepoint at τ).

Note. The point τ is our *changepoint*, e.g. the first point after which our mean changes, however there's a lot of inconsistencies on the literature: sometimes you will find that people refer to $\tau+1$ as the changepoint, and τ as the last pre-change point (as a matter of fact, please let me know if you spot this inconsistency anywhere in these notes!).

To address this problem, one of the most widely used methods is the CUSUM (Cumulative Sum) statistic. The basic idea behind the CUSUM statistic is to systematically compare the distribution of the data to the left and right of each possible changepoint τ . By doing so, we can assess whether there is evidence of a significant change in the mean at a given point.

1.3.1 The CUSUM statistics

The CUSUM statistic works by comparing, for each potential data point, the empirical mean (average) of the data to the left (before τ) with the empirical mean of the data to the right (after τ):

$$C_{\tau} = \sqrt{\frac{\tau(n-\tau)}{n}} \left| \bar{y}_{1:\tau} - \bar{y}_{(\tau+1):n} \right|, \label{eq:ctau}$$

Our $\bar{y}_{1:\tau}$ and $\bar{y}_{(\tau+1):n}$ are just the empirical means of each segment, simply computed with:

$$\bar{y}_{l:u} = \frac{1}{u-l+1} \sum_{t=l}^{u} y_t.$$

The term on the left of the difference, is there to re-scale it so that our statistics is the absolute value of normal RV that has variance 1. If there is no change, this difference is going to be distributed as a standard normal, and this is going to be a key step in drawing the distribution of the CUSUM statistic next week.

This approach is intuitive because if the mean μ is the same across the entire sequence, the values of the averages on both sides of any point τ should be similar. However, if there is a change in the mean, the means will differ significantly, highlighting the changepoint.

More formally, we would detect at change at τ if:

$$\frac{C_{\tau}^2}{\sigma^2} > c,$$

where the $c \in \mathbb{R}^+$ is a suitable chosen threshold value (similar to a critical value in hypothesis testing!).

1.3.2 Algorithmic Formulation of the CUSUM Statistic

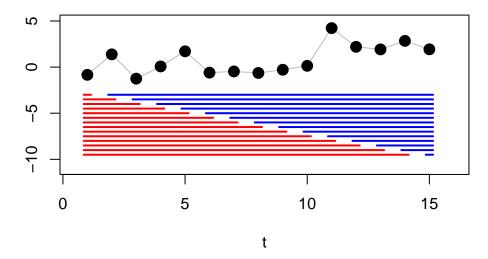
In practice, however, we do not know the changepoint location in advance. Our goal is to detect whether a changepoint exists and, if so, estimate its location. To achieve this, we need to consider all possible changepoint locations and choose the one that maximizes our test statistic.

The natural extension of the likelihood-ratio test to this situation is to use as a test statistic the maximum of C_{τ} as we vary τ :

$$C_{max} = \max_{\tau \in \{1,\dots,n-1\}} C_\tau^2/\sigma^2$$

And detect a changepoint if $C_{max} > c$ for some suitably chosen threshold c. The choice of c will determine the significance level of the test (we'll discuss this in more detail later). Graphically, the test will look:

Cusum over 15 points



If we detect a change point (i.e., if $C_{max} > c$), we can estimate its location by:

$$\hat{\tau} = \arg\max_{\tau \in \{1,\dots,n-1\}} C_{\tau}^2/\sigma^2$$

In other words, $\hat{\tau}$ is the value of τ that maximizes the CUSUM statistic.

A simple estimate of the size of the change is then given by:

$$\Delta \hat{\mu} = \bar{y}_{(\hat{\tau}+1):n} - \bar{y}_{1:\hat{\tau}}$$

This estimate represents the difference between the mean of the data after the estimated changepoint and the mean of the data before the estimated changepoint.

In pseudocode:

INPUT: Time series $y=(y_1,...,y_n)$, threshold c, variance σ . OUTPUT: Changepoint estimate $\hat{\tau}$, maximum CUSUM statistic C_{max}

$$\begin{split} n &\leftarrow \text{length of } y \\ C_{max} &\leftarrow 0 \\ \hat{\tau} &\leftarrow 0 \\ S_n &\leftarrow \sum_{i=1}^n y_i \text{ // Compute total sum of y} \\ S &\leftarrow 0 \end{split}$$

$$\begin{split} & \mathbf{FOR} \ t = 1, \dots, n-1 \\ & S \leftarrow S + y_t \\ & \bar{y}_{1:t} \leftarrow S/t \\ & \bar{y}_{(t+1):n} \leftarrow (S_n - S)/(n-t) \\ & C_t \leftarrow \sqrt{\frac{t(n-t)}{n}} |\bar{y}_{1:t} - \bar{y}_{(t+1):n}| \\ & \mathbf{IF} \ C_t > C_{max} \\ & C_{max} \leftarrow C_t \\ & \hat{\tau} \leftarrow t \end{split}$$

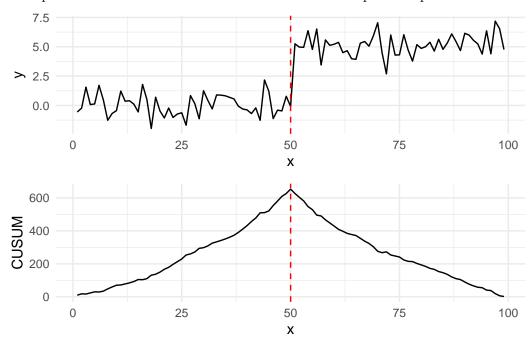
$$\begin{array}{c} \textbf{IF} \ C_{max}^2/\sigma > c \\ \textbf{RETURN} \ \hat{\tau}, \ C_{max} \ // \ \text{Changepoint detected} \\ \textbf{ELSE} \end{array}$$

 $\bf RETURN$ NULL, C_{max} // No changepoint detected

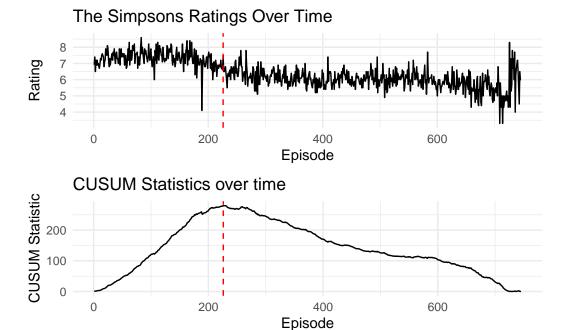
It's worth noting that, as we only need to calculate the CUSUM statistic for each potential changepoint once. By pre-computing the cumulative sum of all observations, this allows. The time complexity of this algorithm is O(n), where n is the length of the time series.

1.3.3 Example

It is possible to see how the cusum behaves on this simple example below:



Running the CUSUM test, and maximising on our Simpsons episode, results in:



This results in episode Thirty Minutes over Tokyo being the last "good" Simpsons episode, with Beyond Blunderdome being the start of the decline, according to the Gaussian change-in-mean model!

1.4 Exercises

1.4.1 Workshop 1

- 1. Determine if the following processes are stationary, piecewise stationary, or non-stationary:
- a. $y_t=y_{t-1}+\epsilon_t, \quad t=2,\dots,n, y_1=0, \epsilon_{1:n}\sim N(0,1).$ Suggestion: try to compute the variance of the process.
- b. $y_t = \epsilon * t + 3 * \cdot \mathbb{1}(t \, 50), \quad t = 1, \dots, 100, \quad \epsilon_{1:100} \sim N(0, 1)$
- c. $y_t = 0.05 \cdot t + \epsilon_t, \ t = 1, \dots, 100, \quad \epsilon_{1:100} \sim N(0, 1)$
- 2. In this exercise we will show that the difference $\bar{y}_{1:\tau} \bar{y}_{(\tau+1):n}$, multiplied by the normalizing constant $1/\sigma^2\sqrt{\frac{\tau(n-\tau)}{n}}$, follows a standard normal distribution. **Hint:**
 - a. Compute the expected value and variance of the difference
 - b. Conclude that if you standardise the sum, this follows a normal distribution.

1.4.2 Lab 1

- 1. Code the CUSUM algorithm for a unknown change location, based on the pseudocode above.
- 2. Modify your function above to output the CUSUM statistics over all ranges of tau, and recreate the Simpsons plot above.

2 Controlling the CUSUM and Other Models

In this chapter, we explore the properties of the CUSUM test for detecting a change in mean, and this will allow us how to determine appropriate thresholds, and explore its properties when a changepoint is present.

We will employ some concepts from asymptotic theory: in time series analysis, an asymptotic distribution refers to the distribution that our test statistic approaches as the length of the time series n becomes very large.

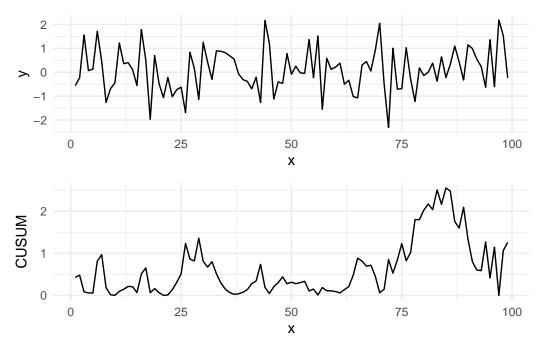
2.1 The asymptotic distribution of the CUSUM statistics

We have learned that the chi-squared distribution is a continuous probability distribution that models the sum of squares of k independent standard normal random variables. More formally, if z_1, \dots, z_k are independent, standard Normal random variables, then:

$$\sum_{i=1}^k z_i^2 \sim \chi_k^2$$

We have met this distribution already in hypothesis testing and constructing confidence intervals. The shape of the distribution depends on its degrees of freedom (k). For k = 1, it's highly skewed, but as k increases, it becomes more symmetric and approaches a normal distribution.

We learned that, when properly normalized C_{τ} follows a standard normal distribution under the null hypothesis of no change. Therefore, our test statistics for a fixed τ , C_{τ}^2/σ^2 , follows a chi-squared distribution with 1 degree of freedom, being the square of a standard random variable. If we take the example of last week, and remove the changepoint, we can observe that the cusum statistics stays constant, and relatively small:



However, as the change is unknown, our actual test statistic for detecting a change is $\max_{\tau} C_{\tau}^2/\sigma^2$.

For this reason, calculating the distribution of this maximum ends up being a bit more challenging...

- 1. So far, we worked only for one fixed τ , however, when comparing the maximums, the values of C_{τ} are in fact not independent across different τ s.
- 2. As we will learn later, the CUSUM is a special case of a LR test, as setting the size of the actual change in mean to 0 effectively removes the changepoint parameter from the model. For this reason, the usual regularity conditions for likelihood-ratio test statistics don't apply here.

2.1.1 Controlling the max of our cusums

Fortunately, for controlling our CUSUM test, we can use the fact that $(C_1, ..., C_{n-1})/\sigma$ are the absolute values of a Gaussian process with mean 0 and known covariance, and there are well known statistical results that can help us in our problem. Yao and Davis (1986), in fact, show that the maximum of a set of Gaussian random variables is known to converge to a Gumbel distribution, described by the following equation:

$$\lim_{n\to\infty} \Pr\{a_n^{-1}(\max_\tau C_\tau/\sigma - b_n) \le u_\alpha\} = \exp\{-2\pi^{-1/2}\exp(-u_\alpha)\},$$

where $a_n=(2\log\log n)^{-1/2}$ and $b_n=a_n^{-1}+0.5a_n\log\log\log n$ are a scaling and a centering constant.

The right side of this equation is the CDF of a Gumbell distribution. As we learned from likelihood inference, to find the threshold c_{α} for a given false probability rate, we first set the right-hand side equal to $1 - \alpha$, and solve for u_{α} . This gives:

$$u_{\alpha} = -\log\left(-\frac{\log(1-\alpha)}{2\pi^{-1/2}}\right).$$

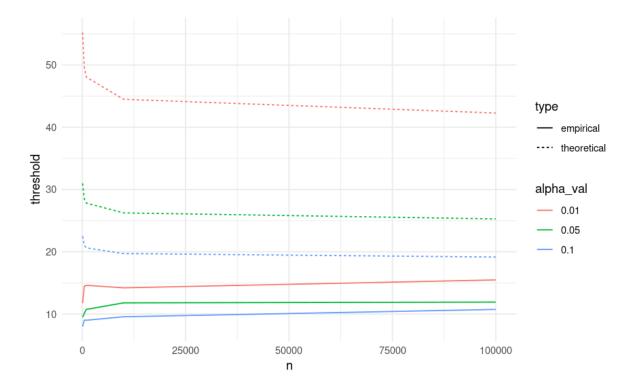
Then, we can find the critical value by looking into the left side of the equation:

$$\tilde{c} = (a_n u_\alpha + b_n),$$

To find the threshold, as $\max_{\tau} \frac{C_{\tau}^2}{\sigma^2} > c$, we just have to square our value above, e.g. $c_{\alpha} = \tilde{c}^2$.

This asymptotic result suggests that the threshold c_{α} for C_{τ}^2/σ^2 should increase with n at a rate of approximately $2 \log \log n$. Given that this is a fairly slow rate of convergence, this suggests that the threshold suggested by this asymptotic distribution can be conservative in practice, potentially leading to detect less changepoints than what actually exist.

In practice, it's often simplest and most effective to use Monte Carlo methods to approximate the null distribution of the test statistic. This approach involves simulating many time series under the null hypothesis (no changepoint) and calculating the test statistic for each. The distribution of these simulated test statistics can then be used to set appropriate thresholds. This, as we will see, it's much better as it ends up having less conservative thresholds:



We will see how to obtain this thresholds in the Lab.

2.2 The Likelihood Ratio Test

The CUSUM can be viewed as a special case of a more general framework based on the Likelihood Ratio Test (LRT). This allow us to test for more general settings, beyond simply detecting changes in the mean.

In general, the Likelihood Ratio Test is a method for comparing two nested models: one under the null hypothesis, which assumes no changepoint, and one under the alternative hypothesis, which assumes a changepoint exists at some unknown position τ .

Suppose we have a set of observations $x_1, x_2, ..., x_n$. Under the null hypothesis H_0 , we assume that all the data is generated by the same model without a changepoint. Under the alternative hypothesis H_1 , there is a single changepoint at τ , such that the model for the data changes after τ . The LRT statistic is given by:

$$LR_{\tau} = -2\log\left\{\frac{\max_{\theta}\prod_{t=1}^{n}L(y_t|\theta)}{\max_{\theta_1,\theta_2}[(\prod_{t=1}^{n}L(y_t|\theta_1))(\prod_{t=1}^{n}L(y_t|\theta_2)]}\right\}$$

{eq-lr-test}

The LRT compares the likelihood of the data under two models to determine which one is more likely: the enumerator, is the likelihood under the null hypothesis of no changepoint, while the denominator represents the likelihood of the data under the alternative hypothesis, where we optimise for two different parameters before and after the changepoint at τ .

2.2.1 Example: Gaussian change-in-mean

The CUSUM statistics, in fact, is nothing but a specific case of this model. To see this, we start from our piecewise costant signal, plus noise, $x_i = f_i + \epsilon_i$, i = 1, ..., n. Under this model our data, a linear combination of a Gaussian, is distributed as:

$$y_i \sim N(\mu_i, \sigma^2), \quad i = 1, \dots, n$$

Therefore, to obtain the likelihood ratio test statistic, we plug our Gaussian kernel into the LR above, and take the logarithm:

$$LR_{\tau} = -2\left[\max_{\mu}\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mu)^2\right) - \max_{\mu_1,\mu_2}\left(-\frac{1}{2\sigma^2}\left(\sum_{i=1}^{\tau}(y_i - \mu_1)^2 + \sum_{i=\tau+1}^{n}(y_i - \mu_2)^2\right)\right)\right]$$

This simplifies to:

$$=\frac{1}{\sigma^2}\left[\min_{\mu}\sum_{i=1}^n(y_i-\mu_1)^2-\min_{\mu_1,\mu_2}\left(\sum_{i=1}^{\tau}(y_i-\mu_1)^2+\sum_{i=\tau+1}^n(y_i-\mu_2)^2\right)\right]$$

To solve the minimization over μ_1 and μ_2 , we plug-in values $\hat{\mu} = \bar{y}_{1:n}$ on the first term, and $\hat{\mu}_1 = \bar{y}_{1:\tau}$, $\hat{\mu}_2 = \bar{y}_{(\tau+1):n}$ for the second term:

$$LR_{\tau} = \frac{1}{\sigma^2} \left[\sum_{i=1}^n (y_i - \bar{y}_{1:n})^2 - \sum_{i=1}^{\tau} (y_i - \bar{y}_{1:\tau})^2 - \sum_{i=\tau+1}^n (y_i - \bar{y}_{(\tau+1):n})^2 \right]$$

This is the likelihood ratio test statistic for a change in mean in a Gaussian model, which is essentially the CUSUM statistics squared, rescaled by the known variance:

$$LR_{\tau} = \frac{C_{\tau}^2}{\sigma^2}$$

This is possible to prove directly after some tedious algebraic manipulations (which we will see in the workshop!).

2.3 Towards More General Models

The great thing of the LR test is that it's extremely flexible, allowing us to detect other changes then the simple change-in-mean case. As before, the procedure is to compute the LR test conditional on a fixed location of a changepoint, e.g. LR_{τ} , and range across all possible values for τ to find the test statistics for our change.

2.3.1 Change-in-variance

To this end we will demostrate how to construct a test for Gaussian change-in-variance, for mean known. For simplicy, we will call our variance $\sigma^2 = \theta$, our parameter of interest, and without loss of generality, we can center our data on zero (e.g. if $x_t \sim N(\mu, \theta)$, then $x_t - \mu = y_t \sim N(0, \theta)$). Then, our p.d.f for one observation will be given by:

$$L(y_t|\theta) = \frac{1}{\theta\sqrt{2\pi}} \exp\{-\frac{y_t}{2\theta}\}.$$

Plugging in the main LR test formula, we find:

$$LR_{\tau} = -2\log\left\{\frac{\max_{\theta}\prod_{t=1}^{n}\frac{1}{\theta\sqrt{2\pi}}\exp\{-\frac{y_{t}}{2\theta}\}}{\max_{\theta_{1},\theta_{2}}[(\prod_{t=1}^{\tau}\frac{1}{\theta\sqrt{2\pi}}\exp\{-\frac{y_{t}}{2\theta}\})(\prod_{t=\tau+1}^{n}\frac{1}{\theta\sqrt{2\pi}}\exp\{-\frac{y_{t}}{2\theta}\})]}\right\}$$

And taking the log, and simplifying over the constant gives us:

$$\min_{\theta} \sum_{t=1}^n \left(\log(\theta) + \frac{y^2}{\theta} \right) - \min_{\theta_1, \theta_2} \left[\ \sum_{t=1}^\tau \left(\log(\theta_1) + \frac{y^2}{\theta_1} \right) + \sum_{t=\tau+1}^n \left(\log(\theta_2) + \frac{y^2}{\theta_2} \right) \right]$$

Now to solve the minimisation, we focus on the first term:

$$f(y_{1:n}, \theta) = \sum_{t=1}^{n} \left(-\log(\theta) - \frac{y^2}{\theta} \right)$$

Simplifying the sum:

$$=\left(-n\log(\theta)-rac{\sum_{t=1}^{n}y^{2}}{\theta}
ight).$$

Taking the derivative with respect to θ , gives:

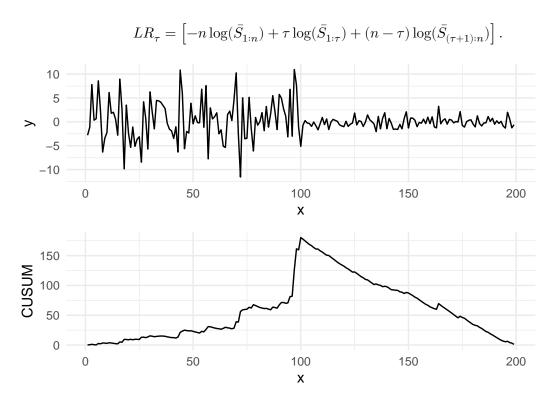
$$\frac{d}{d\theta}f(y_{1:n},\theta) = -\frac{n}{\theta} + \frac{\sum_{t=1}^{n} y^2}{\theta^2}$$

Setting equal to zero and solving for θ :

$$-n\theta + \sum_{t=1}^{n} y^2 = 0$$

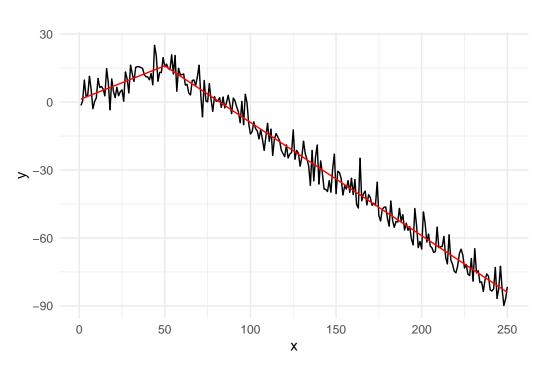
Which gives us: $\hat{\theta} = \frac{\sum_{t=1}^{n} y^2}{n} = \bar{S}_{1:n}$ the sample variance.

Solving the optimization for θ_1 and θ_2 similarly, and plugging in the values $\hat{\theta}_1 = \bar{S}_{1:\tau}$, $\hat{\theta}_2 = \bar{S}_{(\tau+1):n}$, gives us the final LR test:



2.3.2 Change-in-slope

Another important exaple, and an alternative to detecting a change-in-mean, is detecting a change in slope. In this section, we assume the data is still modeled as a signal plus noise, but the signal itself is a linear function of time (e.g. non-stationary, with a change!). Graphically:



More formally, let our data be modeled as:

$$y_t = f_t + \epsilon_t, \quad t = 1, \dots, n,$$

where the noise vector $\epsilon_{1:n} \sim N(0,1)$ consists of independent and identically distributed (i.i.d.) normal random variables. In this scenario, for simplicity, we assume a known constant variance, which without loss of generality, we take to be 1.

Under the null hypothesis H_0 , we assume that the signal is linear with a constant slope over the entire sequence, i.e.,

$$f_t = \theta_0 + t\theta_1, \quad t = 1, \dots, n,$$

where θ_0 is the intercept, and θ_1 is the slope. However, under the alternative hypothesis H_1 , we assume there is a changepoint at τ after which the slope changes. Thus, the signal becomes:

$$f_t = \theta_0 + t\theta_1, \quad t = 1, \dots, \tau; \quad f_t = \theta_0 + \tau\theta_1 + (t-\tau)\theta_2, \quad t = \tau+1, \dots, n,$$

where θ_2 is the new slope after the changepoint. In other words, the model is showing a continuous piecewise linear mean.

For this model, the log-likelihood ratio test statistic can be written as the square of a projection of the data onto a vector v_{τ} , i.e.,

$$LR_{\tau} = (v_{\tau}^{\top} y_{1:n})^{2},$$

where v_{τ} is a contrast vector that is piecewise linear with a change in slope at τ . This vector is constructed such that, under the null hypothesis, the vector $v_{\tau}^{\top}y_{1:n}$ has variance 1, and $v_{\tau}^{\top}y_{1:n}$ is invariant to adding a linear function to the data. These properties uniquely define the contrast vector v_{τ} , up to an arbitrary sign. Computations on how to obtain this likelihood ration test, and how to construct this vector are beyond the scope of this module, but should you be curious those are detailed in Baranowski, Chen, and Fryzlewicz (2019).

2.3.3 Revisiting our Simpsons data (again!)

So, going back to the Simpsons example... We mentioned how the belowed show rose rapidly to success, and at one point, started to *decline*... A much better model would therefore be our change-in-slope model!

To run the model, we can take advantage of the **not** package, which by default is a multiple changepoint algorithm (we will see these in the next week), but whose simplest case implements exactly our change-in-slope LR test.

Before we proceed, we need to load, clean and standardize our data:

```
# Load Simpsons ratings data
simpsons_episodes <- read.csv("extra/simpsons_episodes.csv")
simpsons_episodes <- simpsons_episodes |>
   mutate(Episode = id + 1, Season = as.factor(season), Rating = tmdb_rating)
simpsons_episodes <- simpsons_episodes[-nrow(simpsons_episodes), ]

y <- simpsons_episodes$Rating</pre>
```

We can then run our model with:

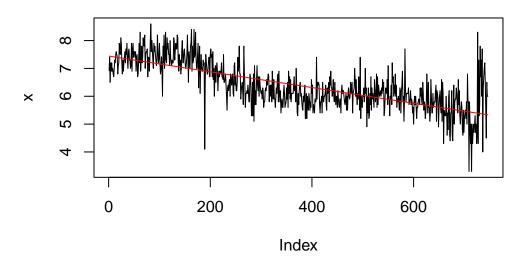
```
library(not)

r <- not(y, method = "max", rand.intervals = FALSE, contrast = "pcwsLinContMean", intervals = print(paste0("Our changepoint estimate: ", features(r)$cpt))</pre>
```

[1] "Our changepoint estimate: NA"

plot(r)

Data and the fitted signal



We notice how the test statistics implemented does not detect any significant change... As this may sound a bit anti-climatic, there is still some relaxation on the hypotheses that we can do to obtain a better answer. We can, in fact, relax the hypothesis that the regression line needs to be continuous, and assume that there might be a change in the intercept too, signifying an abrupt change:

$$f_t=\theta_0+t\theta_1, \quad t=1,\dots,\tau; \quad f_t=\theta_0+\theta_2+\tau\theta_1+(t-\tau)\theta_3, \quad t=\tau+1,\dots,n,$$

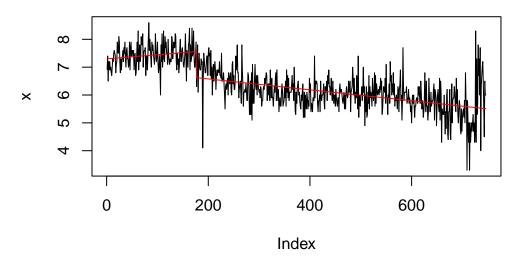
We can do that by changing the model via the contrast argument:

```
r <- not(y, method = "max", rand.intervals = FALSE, contrast = "pcwsLinMean", intervals = rand
print(paste0("Our changepoint estimate: ", features(r)$cpt))</pre>
```

[1] "Our changepoint estimate: 176"

plot(r)

Data and the fitted signal



We can see that we now find a significant changepoint prior to episode The Simpsons Spin-Off Showcase, which is anthology episode well over into season 8, which is by many considered the last good one!

2.4 Exercises

2.4.1 Workshop 2

- 1. Show that the likelihood ratio test statistic for a change in mean in a Gaussian model is the CUSUM statistics squared, rescaled by the known variance, e.g. $LR_{\tau} = C_{\tau}^2/\sigma^2$.
- 2. Compute the LR ratio to detect a change in the success probability of a Bernoulli Random Variable.

2.4.2 Lab 2

- 1. Write a function, that taking as input n and a desired α level for false positive rate, returns the threshold for the cusum statistics.
- 2. Construct a function that, taking as input n, a desired α , and a replicates parameter, runs a Monte Carlo simulation to tune an empirical penalty for the CUSUM change-inmean on a simple Gaussian signal. Tip: You can reuse the function for computing the CUSUM statistics that you built the last week

- 3. Compare for a range of increasingly values of n, e.g. n=100,500,1000,10.000, and for few desired levels of alpha, the Monte Carlo threshold with the theoretically justified threshold. Plot the results, to recreate the plot above.
- 4. Using the Test the Simpsons dataset, find a critical level for your CUSUM statistics, and declare a change with the change-in-mean model.

3 Multiple changepoints

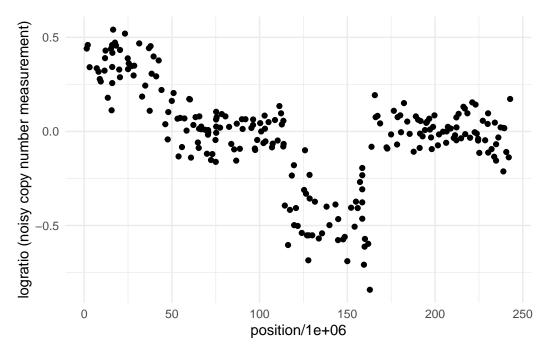
3.1 Introduction

In real-world data, it is common to encounter situations where more than one change occurs. When applying the CUSUM statistic in such cases, where there are **multiple changes**, the question arises: how does CUSUM behave, and how can we detect these multiple changes effectively?

3.1.1 Real Example: Genomic Data and Neuroblastoma

To motivate this discussion, we return to the example from week 1: detecting active genomic regions using *ChIP-seq data*. Our goal here is to identify copy number variations (CNVs)—structural changes in the genome where DNA sections are duplicated or deleted. These variations can impact gene expression and are linked to diseases like cancer, including neuroblastoma. The dataset we'll examine consists of logratios of genomic probe intensities, which help us detect changes in the underlying DNA structure.

Statistically our objective is to segment this logratio sequence into regions with different means, corresponding to different genomic states:



As seen from the plot, the data is noisy, but there are visible shifts in the logratio values, suggesting multiple changes in the underlying copy number. By the end of this chapter, we will segment this sequence!

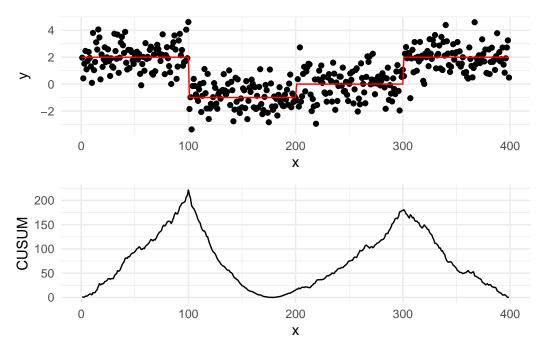
3.1.2 Towards multiple changes

Under this framework, the observed sequence y_t can be modeled as a piecewise constant signal with changes in the mean occurring at each changepoint τ_k . A plausible model for the change-in-mean signal is given by

$$y_t = \mu_k + \epsilon_t, \quad \text{for } \tau_k \leq t < \tau_{k+1}, \ k = 0, 1, \dots, K,$$

where μ_k is the mean of the k-th segment, and $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$ are independent Gaussian noise terms with mean 0 and (known) variance σ^2 .

As a starting example, we can generate a sequence with 4 segments, with $\tau_1 = 50, \tau_2 = 100, \tau_3 = 150$ and means $\mu_1 = 2, \mu_2 = 0, \mu_3 = -1$ and $\mu_4 = 2$. Running the CUSUM statistic in this scenario with multiple changes, leads to the following C_{τ}^2 trace:



From this, we notice that our test still has power to detect some of the changes, but the estimate that we get, is initially wrong. $\Delta \mu = |\mu_1 - \mu_2|$. Is power lost when there is more then one change in our test?

Well, to answer this question, we can compare the values of the CUSUM statistic ran on the whole dataset (as above), with the values of the CUSUM, ran on a subset containing only one change:

Warning: Removed 199 rows containing missing values or values outside the scale range (`geom_line()`).



We can see that max of the old cusum (the line in grey) is much lower than the one where we isolate the sequence on one single change! So there is an effective loss of power in this scenario in analyzing all changes together, as some changes are masking the effects of others...

This gives us motivation to move towards some methodology that tries to estimate all changes locations jointly, rather then one at a time!

3.1.3 The cost of a segmentation

Well, so far we only worked with one scheme that tried to split a sequence in a hald

But how can we work in case we have more than one change? Well, we need to introduce the cost of a segment.

If we assume the data is independent and identically distributed within each segment, for segment parameter θ , then this cost can be obtained through:

$$\mathcal{L}(y_{s+1:t}) = \min_{\theta} \sum_{i=s+1}^{t} -\log(f(y_i, \theta))$$

with $f(y,\theta)$ being the likelihood for data point y if the segment parameter is θ . Now, for example, in the gaussian case this cost is given by:

$$\mathcal{L}(y_{s:t}) = \frac{1}{2\sigma^2} \sum_{i=s}^{t} \left(y_i - \bar{y}_{s:t} \right)^2$$

The cost for the full segmentation will be given by the sum across all segments:

$$\sum_{k=0}^K \mathcal{L}(y_{\tau_k+1:\tau_{k+1}})$$

Interestingly, the cost of a full segmentation is closely related to the LR test. Consider, a single Gaussian change-in-mean at time τ , splitting the data into two segments: $y_{1:\tau}$ and $y_{\tau+1:n}$. The cost of this segmentation is:

$$\mathcal{L}(y_{1:\tau}) + \mathcal{L}(y_{\tau+1:n}) = \frac{1}{\sigma^2} \left[\sum_{i=1}^{\tau} (y_i - \bar{y}_{1:\tau})^2 + \sum_{i=\tau+1}^{n} (y_i - \bar{y}_{(\tau+1):n})^2 \right]$$

Which is essentially the same LR test as we saw last week, without the null component. Specifically, for one change, minimizing the segmentation cost over all possible changepoints locations τ is equivalent to maximizing the CUSUM statistic.

3.1.4 The "best" segmentation

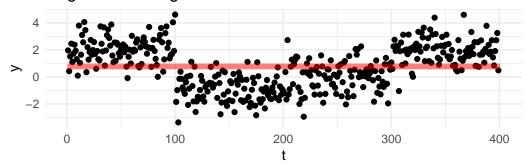
We now have a way of evaluating how "good" a segmentation is, so it's only natural to ask the question: what would be the best one?

Well, one way would be to, say, finding the the best set of $\tau = \tau_0, \dots, \tau_{K+1}$ changepoints that minimise the cost:

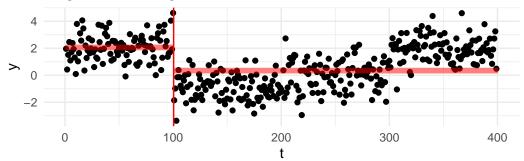
$$\min_{\substack{K \in \mathbb{N} \\ \tau_1, \dots, \tau_K}} \sum_{k=0}^K \mathcal{L}(y_{\tau_k+1:\tau_{k+1}}). \tag{3.1}$$

Which one would this be? Say that for instance we range the K = 1, ..., n, and at each step we find the best possible segmentation. Graphically, we would be observing the following:

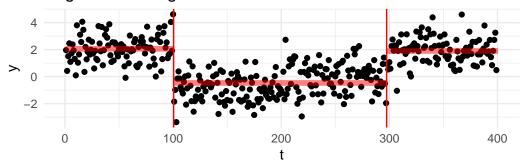




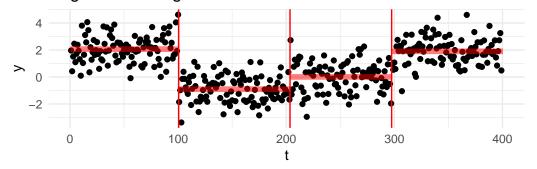
Segments: 2 Seg. Cost: 821



Segments: 3 Seg. Cost: 441

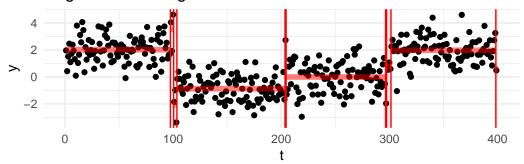


Segments: 4 Seg. Cost: 400

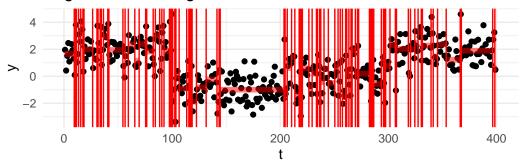


Well, arguably we would like to stop at 4, which we know is the real number of segments, but the cost keep going down...

Segments: 10 Seg. Cost: 369

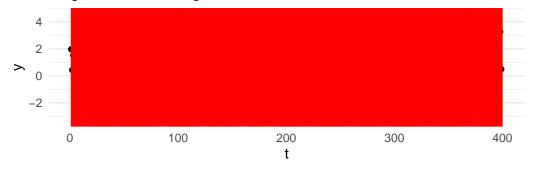


Segments: 100 Seg. Cost: 133



And finally:

Segments: 400 Seg. Cost: 0





Well, it turns out, that according to the minimization above, the optimal segmentation across all would be the one that puts each point into its own segment!

Well, there are different solutions to this problem. The first one we will see, is a divideand-conquer greedy approach, called Binary Segmentation, and the second one will aim a generating a different optimization to the one below that will find the optimal segmentation up to a constant to avoid over-fitting!

3.2 Binary Segmentation

Binary Segmentation (BS) is a procedure from ? and ?. Binary segmentation works like this:

1. Start with a test for a change τ that splits a sequence into two segments and to check if the cost over those two segments, plus a penalty $\beta \in \mathbb{R}$, is smaller then the cost computed on the whole sequence:

$$\mathcal{L}(y_{1:\tau}) + \mathcal{L}(y_{\tau+1:n}) + \beta < \mathcal{L}(y_{1:n}) \tag{3.2}$$

where the segment cost $\mathcal{L}(\cdot)$, is as in Equation 3.1.

2. If the condition in Equation 3.2 is true for at least one $\tau \in 1, ..., n$, then the τ that minimizes $\mathcal{L}(y_{1:\tau}) + \mathcal{L}(y_{\tau+1:n})$ is picked as a first changepoint and the test is then performed

on the two newly generated splits. This step is repeated until no further changepoints are detected on all resulting segments.

3. If there are no more resulting valid splits, then the procedure ends.

Some of you might have noted how the condition in Equation 3.2 is closely related to the LR test in ?@eq-lr-test. In fact, rearranging equation above, gives us:

$$-\mathcal{L}(y_{1:n}) + \mathcal{L}(y_{1:\tau}) + \mathcal{L}(y_{\tau+1:n}) = -\frac{LR_{\tau}}{2} < -\beta.$$

The $-\beta$ acts exactly as the constant c for declaring a change, and it adds a natural stopping condition, solving the issue of overfitting that we mentioned in the previous section! Binary Segmentation, in fact, does nothing more then iteratively running a LR test, until no changes are found anymore!

This gives us a strategy to essentially apply a test that is locally optimal for one change, such as the Likelihood Ratio test, to solve a multiple changepoint segmentation. For this reason, BS is often employed to extend single changepoint procedures to multiple changes procedures, and hence it is one of the most prominent methods in the literature.

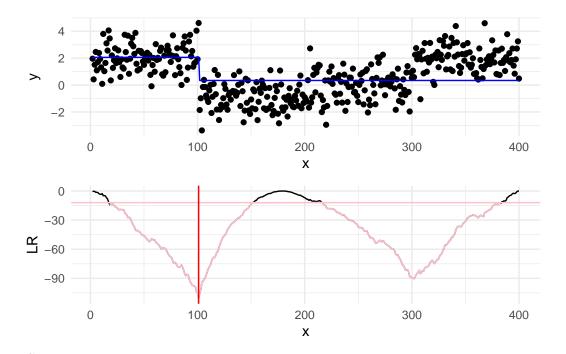
3.2.1 Binary Segmentation in action

Having introduced the main idea, we show now how binary segmentation works in action with an example above. Say that we set a $\beta = 2 \log(400) = 11.98$.

Step 1: We start by computing the cost as in Equation 3.2, and for those that are less then β , we pick the smallest. This will be our first changepoint estimate, and the first point of split.

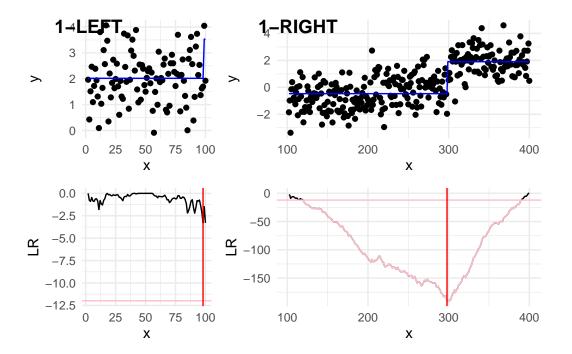
In the plots below, the blue horizontal line is the mean signal estimated for a given split, while in the cusum the pink will represent the values of the LR below the threshold β , and red vertical line will show the min of the test statistics. When the cost is below the beta line, this will be our changepoint estimate.

In our case, we can see that the min of our cost has been achieved for $\hat{\tau} = 100$, and since this is below the threshold, it's our first estimated changepoint!



Step 2: From the first step, we have to check now two splits:

- The first left split, **1-LEFT** in the plot below, covers data $y_{1:100}$. We can see that from here, the min of our statistic is below the threshold, therefore we won't declare any further change in this subset.
- The first right split, **1-RIGHT** covers data $y_{101:400}$. We can see that here, the min of the statistics, is below the threshold, and therefore we identify a second change at $\hat{\tau} = 297$. This is not exactly 300, so we don't have a perfect estimate. Despite this is not ideal, this is the best point we have found and therefore we have to continue!



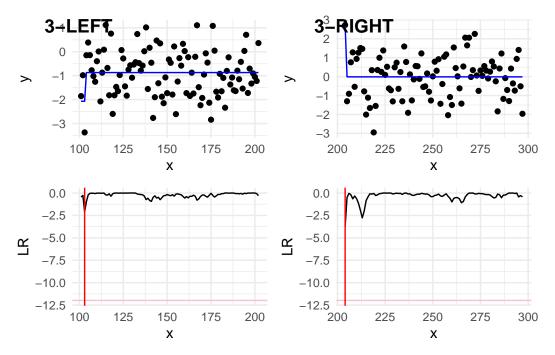
Step 3: In step 3, we have to check again two splits splits:

- The second left split, **2-LEFT** in the plot below, covers data $y_{101:297}$. Now, it's in this split that the statistics goes below the threshold! The third estimated change is at $\hat{\tau} = 203$, again slightly off the real one at 200. We continue investigating this split...
- The second right split, **2-RIGHT** covers data $y_{298:400}$. In this last split, the min is not over the threshold, therefore we stop the search.



Step 4: In step 4, we check:

- The third left split, **3-LEFT** in the plot below, covers data $y_{101:203}$. The minimum, in here is not over the threshold.
- The third right split, **3-RIGHT** covers data $y_{204:298}$. Similarly, the minimum is not over the treshold.



The algorithm therefore terminates!

With this graphical description in mind, we formally describe the Binary Segmentation algorithm as a recursive procedure, where the first iteration would be simply given by $\operatorname{BinSeg}(y_{1:n},\beta)$.

 $BinSeg(y_{s:t}, \beta)$

INPUT: Subseries $y_{s:t} = \{y_s, \dots, y_t\}$ of length t-s+1, penalty β **OUTPUT:** Set of detected changepoints cp

IF $t - s \le 1$

RETURN {} // No changepoint in segments of length 1 or less

COMPUTE

$$\mathcal{Q} \leftarrow \min_{\tau \in \{s, \dots, t\}} \left[\mathcal{L}(y_{s:\tau}) + \mathcal{L}(y_{\tau+1:t}) - \mathcal{L}(y_{s:t}) + \beta \right]$$

IF Q < 0

$$\begin{split} \hat{\tau} \leftarrow & \underset{\tau \in \{s, \dots, t\}}{\min} \left[\mathcal{L}(y_{s:\tau}) + \mathcal{L}(y_{\tau+1:t}) - \mathcal{L}(y_{s:t}) \right] \\ cp \leftarrow & \{\hat{\tau}, \mathrm{BinSeg}(y_{s:\hat{\tau}}, \beta), \mathrm{BinSeg}(y_{\hat{\tau}+1:t}, \beta) + \hat{\tau} \} \\ \mathbf{RETURN} \ cp \end{split}$$

RETURN {} // No changepoint if -LR/2 is above penalty $-\beta$

3.3 Optimal Partitioning

Another solution to avoid the over-fitting problem of Equation 3.1 lies in introducing a penalty term that discourages too many changepoints, avoiding overfitting. This is known as the penalised approach.

To achieve this, we want to minimize the following cost function:

$$Q_{n,\beta} = \min_{K \in \mathbb{N}} \left[\min_{\tau_1, \dots, \tau_K} \sum_{k=0}^K \mathcal{L}(y_{\tau_k + 1: \tau_{k+1}}) + \beta K \right],$$

where $Q_{n,\beta}$ represents the optimal cost for segmenting the data up to time n with a penalty \$ that increases with each additional changepoint K. With the β term, for every new changepoint added, the cost of the full segmentation increases, discouraging therefore models with too many changepoints.

Unlike Binary Segmentation, which works iteratively and makes local decisions about potential changepoints, and as we have seen it is prone to errors, solving $Q_{n,\beta}$ ensures that the segmentation is **globally optimal**, as in the location of the changes are the best possible to minimise our cost.

Now, directly solving this problem using a brute-force search is computationally prohibitive, as it would require checking every possible combination of changepoints across the sequence: the number of possible segmentations grows exponentially as n increases...

Fortunately, this problem can be solved efficiently using a sequential, dynamic programming algorithm: **Optimal Partitioning (OP)**, from Jackson et al. (2005). OP solves **?@eq-pen-cost** exactly through the following recursion.

We start with $\mathcal{Q}_{0,\beta} = -\beta$, and then, for each t = 1, ..., n, we compute:

$$\mathcal{Q}_{t,\beta} = \min_{0 \leq \tau < t} \left[\mathcal{Q}_{\tau,\beta} + \mathcal{L}(y_{\tau+1:t}) + \beta \right]. \tag{3.3}$$

Here, $\mathcal{Q}_{t,\beta}$ represents the optimal cost of segmenting the data up to time t. The algorithm builds this solution sequentially by considering each possible segmentation $\mathcal{Q}_{0,\beta},\,\cdots,\mathcal{Q}_{t-2,\beta},\,\mathcal{Q}_{t-1,\beta}$ before the current time t, plus the segment cost up to current time t, $\mathcal{L}(y_{\tau+1:t})$.

3.3.1 Optimal partitinioning in action

This recursion can be quite hard to digest, and is, as usual, best described graphically.

Step 1 Say we are at t = 1. In this case, according to equation above, the optimal cost up to time one will be given by (remember that the β cancels out with $Q_{0,\beta}!$):

$$\mathcal{Q}_{1,\beta} = [-\beta + \mathcal{L}(y_{1:1}) + \beta] = \mathcal{L}(y_{1:1})$$



Step 2. Now, at the second step, we have to minimise between two segmentations:

- One with the whole sequence in a second segment alone (again, β cancels out with $Q_{0,\beta} = -\beta$), and this will be given by $\mathcal{L}(y_{1:2})$ (dotted line)
- One with the optimal segmentation from step 1 $\mathcal{Q}_{1,\beta}$ (whose cost considered only the first point in its own segment!), to which we have to sum the cost relative to a second segment $\mathcal{L}(y_{2:2})$ that puts the second point alone, and the penalty β as we have added a new segment!

We minimise across the two, and this gives us $Q_{2,\beta}$.



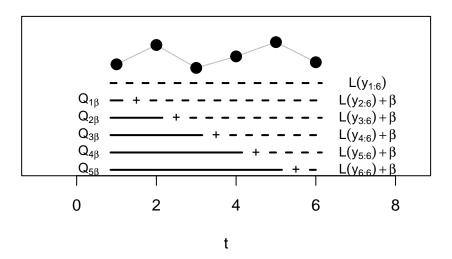
Step 3: Similarly, at t=3 we have now three segmentations to choose from:

- The one that puts the first three observations in the same segment, whose cost will be given simply by $\mathcal{L}(y_{1:2})$,
- The one considering the optimal segmentation from time 1, plus the cost of adding an extra segment with observation 2 and 3 together
- Finally the optimal from segmentation 2, $\mathcal{Q}_{2,\beta}$, plus the segment cost of fitting an extra segment with point 3 alone. Note that $\mathcal{Q}_{2,\beta}$ will come from the step before: if we would have been beneficial to add a change, at the previous step, this information is carried over!

Again, we pick the minimum across these three to get $\mathcal{Q}_{3,\beta}$, and proceed.



Step n Until the last step! Which would look something like this:



A formal description of the algorithm can be found below:

INPUT: Time series $y = (y_1, ..., y_n)$, penalty β **OUTPUT:** Optimal changepoint vector cp_n

 $\begin{array}{l} \text{Initialize } \mathcal{Q}_0 \leftarrow -\beta \\ \text{Initialize } cp_0 \leftarrow \{\} \end{array}$

$$\begin{split} \mathbf{FOR} \ t &= 1, \dots, n \\ \mathcal{Q}_t \leftarrow \min_{0 \leq \tau < t} \left[\mathcal{Q}_\tau + \mathcal{L}(y_{\tau+1:t}) + \beta \right] \\ \hat{\tau} \leftarrow \arg\min_{0 \leq \tau < t} \left[\mathcal{Q}_\tau + \mathcal{L}(y_{\tau+1:t}) + \beta \right] \\ cp_t \leftarrow \left(cp_{\hat{\tau}}, \hat{\tau} \right) / \text{Append the changepoint to the list at the last optimal point} \end{split}$$

RETURN cp_n

Running the Optimal Partitioning method on our example scenario, with the same penalty $\beta = 2\log(400) = 11.98$ as above, gives changepoint locations $\tau_{1:4} = \{100, 203, 301\}$.

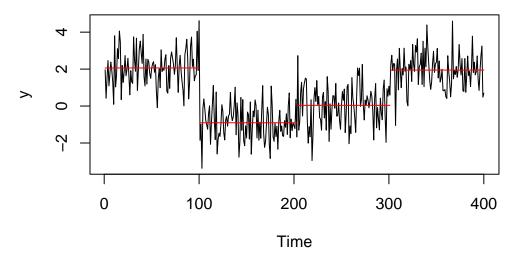
Loading required package: zoo

Attaching package: 'zoo'

The following objects are masked from 'package:base':

as.Date, as.Date.numeric

Successfully loaded changepoint package version 2.2.4 See NEWS for details of changes.

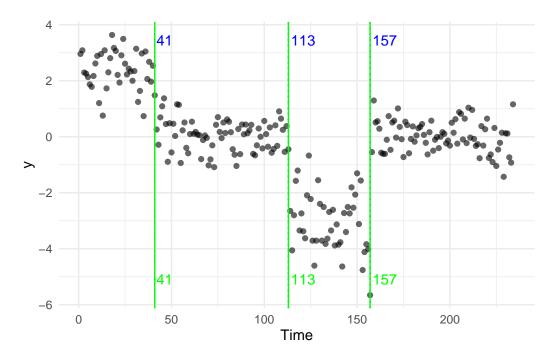


So we can see how on this dataset in particular, OP performs slightly better then Binary Segmentation on the last change, getting closer to the real changepoint of 300!

3.3.2 Neuroblastoma example

Returning to the original example at the start of the module, the neuroblastoma dataset, we run both Binary Segmentation, and Optimal Partitioning.

We report results in the plot below (blue for BS, green for OP). In this case, the algorithms return the same four changepoints:



Some of you might come up with two (very interesting) questions that hopefully we will answer next week...

- If the methods perform roughly the same, which one do I choose?
- Why is the data on a different scale then that presented at the start of the chapter?

3.4 Exercises

3.4.1 Workshop 3

1. For the vector $y_{1:4} = \{0.5, -0.1, 12.1, 12.4\}$, and a penalty $\beta = 5$ calculate, pen on paper (and calculator), all the Binary Segmentation, and Optimal Partitioning steps. **TIP**: To speed up computations, you want to pre-compute all segment costs $\mathcal{L}(y_{l:u})$. I have pre-computed some of these costs in the table below:

$l \backslash u$	1	2	3	4
1	$\mathcal{L}(y_{1:1})$	0.18	94.59	145.43
2		0.00	$\mathcal{L}(y_{2:3})$	101.73
3			0.00	$\mathcal{L}(y_{3:4})$
4				0.00

3.4.2 Lab 3

- 1. Code the Optimal Partitioning algorithm for the Gaussian change-in-mean case. **Tips:**
 - a. Again, you can pre-compute all the possible $\mathcal{L}(y_{l:u})$, for $u \geq l$ to save computational time
 - b. Be very careful with indexing... R starts indexing at 1, however, in the pseudocode, you have one element that starts at 0...
- 2. Install the changepoint package. The example signal of Section 3.4, with the same penalty value of $\beta = 2 * log(n)$, compare your implementation of OP, Binary Segmentation, and PELT. You will learn how to do so in the documentation, running ?cpt_mean. You should make 300 replicates each of your experiment, and compare:
 - a. The absolute error loss from the mean signal, e.g. $||\mu_{1:n} \hat{\mu}_{1:n}||_2^2$
 - b. The absolute error in the number of change points reconstructed, e.g. $|K-\hat{K}|$. What do we observe?
 - c. The runtime for one sequence of PELT agains Binary Segmentation. Evaluate the runtime with package microbenchmark.

4 PELT, WBS and Penalty choices

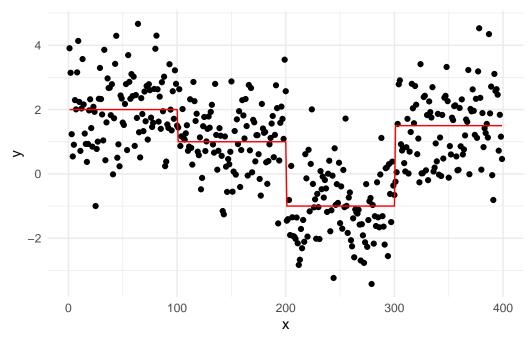
4.1 Drawbacks of OP and BS

When deciding which segmentation approach to use, Binary Segmentation (BS) and Optimal Partitioning (OP) each offer different strengths. The choice largely depends on the characteristics of the data and the goal of the analysis.

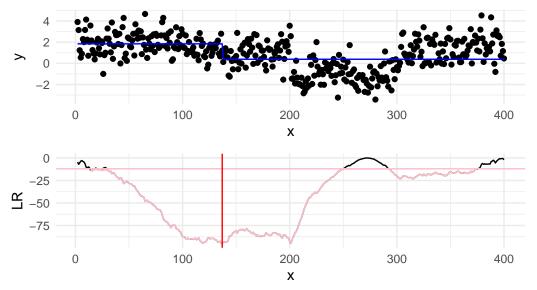
4.1.1 Quality of the Segmentation

Generally, Optimal Partitioning (OP) provides the *most accurate segmentation*, especially when we have a well-defined model and expect precise changepoint detection. OP ensures that the solution is optimal by globally minimizing the cost function across all possible segmentations. This is ideal for datasets with clear changes, even if noise is present.

Let's consider a case with true changepoints at $\tau=100,200,300,$ and segment means $\mu_{1:4}=2,1,-1,1.5:$

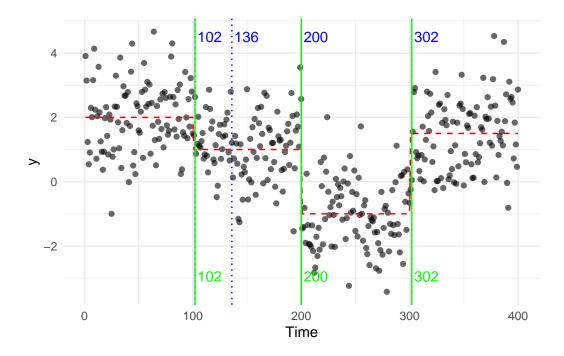


While the underlying signal follows these clear shifts, noise complicates segmentation. Binary Segmentation uses a greedy process where each iteration looks for the largest changepoint. Although fast, this local search can make mistakes if the signal isn't perfectly clear, particularly in the early stages of the algorithm. For example, running BS on this dataset introduces a mistake at $\tau=136$, as shown in the plot below:



This error is carried in the subsequent steps, and the full binary segmentation algorithm will output an additional change at $\tau=136$... Optimal Partitioning (OP), on the other hand, evaluates all possible segmentations considers the overall fit across the entire sequence. It is therefore less susceptible to adding "ghost" changepoints, as rather than focusing on the largest change at each step.

To illustrate, we compare the segmentations generated by both approaches:



4.1.2 Computational Complexity

Well, you may ask why not using OP all the time, then? Well, in changepoint detection, in which is the most appropriate method, we often have to keep track of the computational performance too, and Binary Segmentation is faster on average. For this reason, for large datasets where approximate solutions are acceptable, it might be the best option.

Specifically:

- Binary Segmentation starts by dividing the entire sequence into two parts, iteratively applying changepoint detection to each segment. In the average case, it runs in $\mathcal{O}(n \log n)$ because it avoids searching every possible split point. However, in the worst case (if all data points are changepoints), the complexity can degrade to $\mathcal{O}(n^2)$, as each step can require recalculating test statistics for a growing number of segments.
- Optimal Partitioning, on the other hand, solves the changepoint problem by recursively considering every possible split point up to time t. The result is an optimal segmentation, but at the cost of $\mathcal{O}(n^2)$ computations. This holds true for both the average and worst cases, as it always requires a full exploration of all potential changepoints.

4.2 PELT and WBS

Good news is, despite both algorithms have drawbacks, following *recent developments*, those have been solved. In the next sections, we will introduce two new algorithms, PELT and WBS.

4.2.1 PELT: an efficient solution to OP

In OP, we can reduce the numbers of checks to be performed at each iteration, reducing the complexity. This operation is called *pruning*. Specifically, on the condition that there exists a constant κ such that for every l < t < u:

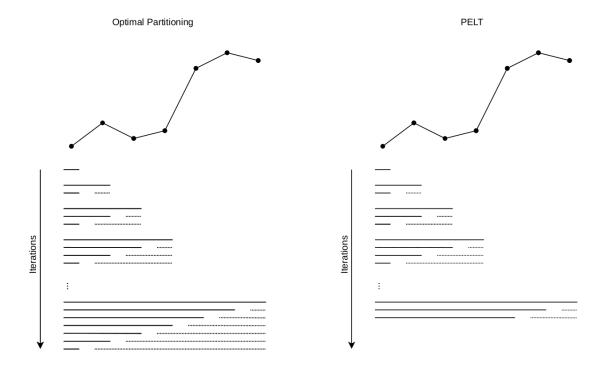
$$\mathcal{L}(y_{l+1:t}) + \mathcal{L}(y_{t+1:u}) + \kappa \le \mathcal{L}(y_{l+1:u})$$

It is possible to prune without resorting to an approximation. For many cost functions, such as the Gaussian cost, such a constant exists. Equating κ to the penalty β , gives us a computational trick to improve on the efficiency... The PELT algorithm – acronym for Pruned Exact Linear Time – (Killick, Fearnhead, and Eckley (2012)) solves exactly the penalised minimization of Equation 3.3 with an expected computational cost that can be linear in n – while still retaining $\mathcal{O}(n^2)$ computational complexity in the worst case. This is achieved by reducing the number of segment costs to evaluate at each iteration via an additional pruning step based on Condition Equation 3.3. That is, if

$$Q\tau + \mathcal{L}(y_{\tau+1:t}) + \kappa \ge Q_t$$

then we can safely prune the segment cost related to τ , as τ will never be the optimal changepoint location up to any time T > t in the future.

The intuition, is that, when $\kappa = \beta$, our penalty, then we would prune at every change detected. And if the changes increase linearly with the length of the data, this means that our algorithm will achieve a $\mathcal{O}(n \log n)$ computational complexity, without any drawbacks!



To reduce computational complexity, we can slightly modify the OP algorithm, to add the pruning condition above:

PELT

INPUT: Time series $y=(y_1,...,y_n)$, penalty β **OUTPUT:** Optimal changepoint vector cp_n

$$\begin{split} \text{Initialize } \mathcal{Q}_0 \leftarrow -\beta \\ \text{Initialize } cp_0 \leftarrow \{\} \\ \text{Initialise } R_1 = \{0\} \end{split}$$

$$\begin{aligned} & \mathbf{FOR} \ t = 1, \dots, n \\ & \mathcal{Q}_t \leftarrow \min_{\tau \in R_t} \left[\mathcal{Q}_\tau + \mathcal{L}(y_{\tau+1:t}) + \beta \right] \\ & \hat{\tau} \leftarrow \arg\min_{\tau \in R_t} \left[\mathcal{Q}_\tau + \mathcal{L}(y_{\tau+1:t}) + \beta \right] \\ & cp_t \leftarrow (cp_{\hat{\tau}}, \hat{\tau}) \ / / \ \text{Append the changepoint to the list at the last optimal point} \\ & R_{t+1} \leftarrow \left\{ \tau \in \left\{ R_t \cup \left\{ t \right\} \right\} : \mathcal{Q}_\tau + \mathcal{L}(y_{\tau+1:t}) + \beta \leq \mathcal{Q}_t \right\} \ / / \ \text{prune the non-optimal changepoint locations} \end{aligned}$$

RETURN cp_n

As the segmentation retained is effectively the same, there are literally no disadvantages in using PELT over OP, if the cost function allows to do so.

However, PELT still has some disadvantages:

- PELT pruning works only over some cost functions, those for which the condition above is true. For example, in the continuous change-in-slope case, we have that the cost from the next change depends on the location of the previous one, making it impossible for PELT to prune without loosing optimality.
- We mentioned above how PELT over iterations at which a change is detected. For signals where changes are not frequent, PELT does not benefits from. A more sophisticated approach is that of **FPOP**, that prunes at every iteration. FPOP employs a different type of pruning, called functional pruning, that at every iteration only check costs that are likely associated to a change. However, despite the pruning is stronger FPOP works only over few selected models.

4.2.2 WBS: Improving on Binary Segmentation

In BS, one of the issues that may arise, is an incorrect segmentation. WBS, Fryzlewicz (2014), is a multiple changepoints procedures that improve on the BS changepoint estimation via computing the initial segmentation cost of BS multiple times over M+1 random subsets of the sequence, $y_{s_1:t_1},\ldots,y_{s_M:t_M},y_{1:n}$, picking the best subset according to what achieves the smallest segmentation cost and reiterating the procedure over that sample accordingly. The idea behind WBS lies in the fact that a favorable subset of the data $y_{s_m:t_m}$ could be drawn which contains a true change sufficiently separated from both sides s_m,t_m of the sequence. By the inclusion of the $y_{1:n}$ entire sequence among the subsets, it is guaranteed that WBS will do no worse than the simple BS algorithm.

We can formally provide a description of WBS as a recursive procedure again, just adding a couple of alterations to the original Binary Segmentation:

$\text{WBS}(y_{s:t},\beta)$	

INPUT: Subseries $y_{s:t} = \{y_s, \dots, y_t\}$ of length t - s + 1, penalty β **OUTPUT:** Set of detected changepoints cp

IF $t-s \leq 1$

RETURN {} // No changepoint in segments of length 1 or less

Draw $\mathcal{M} = \{[s_1, t_1], \dots, [s_M, t_M]\}$ tuples of subset indexes; $\mathcal{M} \leftarrow \mathcal{M} \cup \{[1, n]\}$ **COMPUTE**

$$\mathcal{Q} \leftarrow \min_{\substack{[s_m,t_m] \in \mathcal{M} \\ \tau \in \{s_m,\dots,t_m\}}} \left[\mathcal{L}(y_{s:\tau}) + \mathcal{L}(y_{\tau+1:t}) - \mathcal{L}(y_{s:t}) + \beta \right]$$

$$\begin{split} \mathbf{IF} \ \mathcal{Q} &< 0 \\ \hat{\tau} \leftarrow \underset{\substack{[s_m,t_m] \in \mathcal{M} \\ \tau \in \{s_m,\dots,t_m\}}}{\text{arg min}} \left[\mathcal{L}(y_{s:\tau}) + \mathcal{L}(y_{\tau+1:t}) - \mathcal{L}(y_{s:t}) \right] \\ cp \leftarrow \left\{ \hat{\tau}, \text{WBS}(y_{s:\hat{\tau}},\beta), \text{WBS}(y_{\hat{\tau}+1:t},\beta) + \hat{\tau} \right\} \\ \mathbf{RETURN} \ cp \end{split}$$

RETURN {} // No changepoint if -LR/2 is above penalty $-\beta$

One of the major drawbacks of WBS is that in scenarios where we find frequent changepoints, in order to retain a close-to-optimal estimation, one should draw a higher number of M intervals (usually of the order of thousands of intervals). This can be problematic given that WBS has computational complexity that grows linearly in the total length of the observations of the subsets.

4.3 Penalty Selection

In previous sections, we applied the changepoint detection algorithms using a penalty term of $2\log(n)$. As we'll see, this is the **BIC penalty** (Bayes Information Criterion), a widely used penalty in changepoint detection. However, it is important to note that BIC is just one of several penalty types that can be applied...

As in the single change, some penalty may be more conservative then others! Choosing the correct penalty is key to obtaining a sensible segmentation of the data. The penalty term plays a significant role in balancing the goodness-of-fit of the model with its complexity:

 A lower penalty may lead to an over-segmentation, where too many changepoints are detected • A higher penalty could under-segment the data, missing important changepoints.

The three most common penalties, are:

- AIC (Akaike Information Criterion): The AIC penalty takes value of 2p, where p is the number of parameters that one adds to the model. In multiple changes scenario, every new change, we add a new parameter to the model (as we estimate the signal). This, in OP and BS approaches, where the penalty is added at different iterations, shouls we fit a change, this translates in $\beta = 2 \times 2 = 4$ as our β . While simple to apply, AIC is known to be asymptotically inconsistent: it tends to overestimate the number of changepoints as the sample size increases. Intuitively, this is because AIC is designed to minimize the prediction error rather than to identify the true model structure. It favors models that fit the data well, often leading to the inclusion of more changepoints than necessary.
- BIC (Bayesian Information Criterion): The BIC penalty is given by $p \log(n)$. In our approaches, this translates to: $\beta = 2\log(n)$, that we add for each additional changepoint. BIC is generally more conservative than AIC and is consistent, meaning it will not overestimate the number of changepoints as the sample size grows.
- MBIC (Modified BIC): The MBIC penalty, from Zhang and Siegmund (2007), is an extension of the BIC that includes an extra term to account for the spacing of the changepoints. We can approximate it, in practice, by using a value of $\beta = 3\log(n)$ as our penalty. In practice, it is even more conservative then the BIC penalty.

4.3.1 Example in R: Comparing Penalties with PELT

Let's now examine how different penalties impact the results of changepoint detection using the changepoint package in R. We'll focus on the PELT method and compare the outcomes when using AIC, BIC, and MBIC penalties.

As a data sequence, we will pick a different chromosome in our Neuroblastoma dataset. Can you tell, by eye, how many changes are in this sequence?



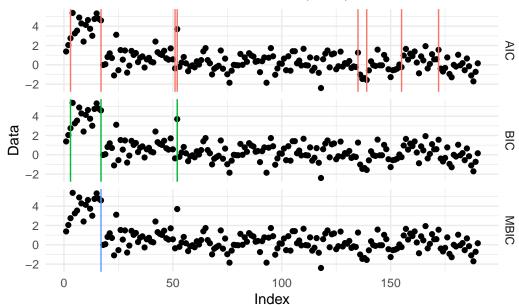
We can compare the three penalties using the changepoint library, as below:

```
data <- one.dt$logratio</pre>
n <- length(data)</pre>
# Apply PELT with AIC, BIC, and MBIC penalties
cp_aic <- cpt.mean(data, method = "PELT", penalty = "AIC")</pre>
cp_bic <- cpt.mean(data, method = "PELT", penalty = "BIC")</pre>
cp_mbic <- cpt.mean(data, method = "PELT", penalty = "MBIC")</pre>
# Extract changepoint locations for each penalty
cp_aic_points <- cpts(cp_aic)</pre>
cp_bic_points <- cpts(cp_bic)</pre>
cp_mbic_points <- cpts(cp_mbic)</pre>
# Create a data frame for plotting with ggplot2
plot_data <- data.frame(</pre>
  index = 1:n,
  data = data)
# Create data frames for changepoints with corresponding method labels
cp_df <- bind_rows(</pre>
  data.frame(index = cp_aic_points, method = "AIC"),
  data.frame(index = cp_bic_points, method = "BIC"),
```

```
data.frame(index = cp_mbic_points, method = "MBIC")
)

ggplot(plot_data, aes(x = index, y = data)) +
    geom_point() + # Plot the data line first
    geom_vline(data = cp_df, aes(xintercept = index, color = method)) +
    facet_grid(method ~ .) +
    labs(title = "PELT with Different Penalties: AIC, BIC, MBIC", x = "Index", y = "Data") +
    theme_minimal() +
    theme(legend.position = "none")
```

PELT with Different Penalties: AIC, BIC, MBIC



We can see how from this example, the AIC likely overestimated the number of changepoints, while BIC and MBIC provided more conservative and reasonable segmentations. By eye, the MBIC seems to have done the better job!

4.3.2 CROPS: running with multiple penalties

Hopefully, the example above should have highlighted that finding the right penalty can be tricky. One solution, would be to run our algorithm for a range of penalties, and then choose a posteriori what the best segmentation is. The CROPS algorithm, from Haynes, Eckley, and Fearnhead (2017), is based on this idea. CROPS works alongside an existing penalised changepoint detection algorithm, like PELT or WBS: as long as the changepoint method can map a penalty value to a (decreasing) segmentation cost, CROPS could be applied.

CROPS takes as input a range of penalties $[\beta_{\min}, \beta_{\max}]$, and explores all possible segmentations within those two penalties in a clever way, to fit the changepoint model as least as we can. As CROPS calculates changepoints for a particular penalty, it keeps track of the range of penalty values where that specific set of changepoints is valid. This works because, for certain ranges of penalties, the set of changepoints stays the same.

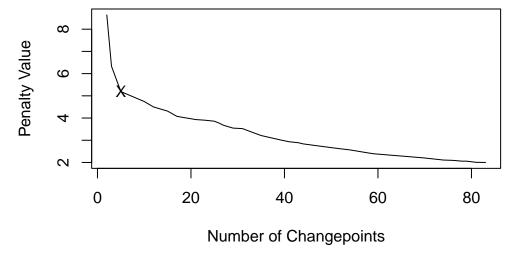
E.g. for penalties between β_1 and β_2 , the changepoints might remain the same, so CROPS only needs to run the changepoint detection once for that range.

We won't introduce the method formally, but in an intuitive way, CROPS works in this way:

- 1. It starts calculates changepoints at two extreme penalties: β_{\min} and β_{\max} . If those are the same, it quits.
- 2. Alternatively, as a binary search, CROPS selects a mid-point penalty $\beta_{\rm int}$ based on whether the segmentation change, and runs the changepoint detection again on $[\beta_{\rm min}, \beta_{\rm int}]$, and $[\beta_{\rm int}, \beta_{\rm max}]$, refining its search for the next penalty.
- 3. It repeats 2 iteratively until no further segmentations are found.

We can use CROPS to generate an **elbow plot** for selecting the appropriate penalty value in changepoint detection. In Data Science and Machine Learning, elbow plots are graphs that helps us choosing the appropriate value of a parameter, balancing between model complexity (in our case number of changepoints) and goodness of fit (how tightly our model fits the data).

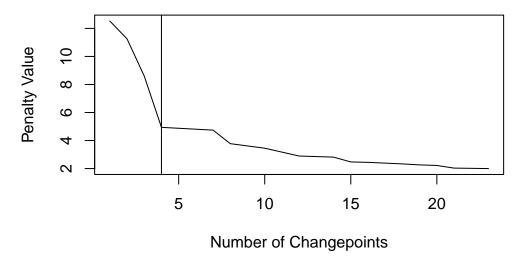
In case of CROPS, we can plot the penalty value from our range, against the number of changepoints. The curve typically shows a steep drop at first, as many changepoints are detected with low penalties, then flattens as the penalty increases and fewer changepoints are added. The **elbow** (hence its name) is the point where the rate of change in the number of changepoints significantly slows down:



The elbow is a point of balance between model fit and complexity. As a rule of thumb, a good choices of a penalty reside in picking either the penalty that generates the segmentation at the elbow, or the one at the point immediately prior.

Going back to our neuroblastoma example above. We run CROPS for penalties [2, 40], and we then generate the elbow plot:

```
out <- cpt.mean(data, method = "PELT", penalty = "CROPS", pen.value = c(2, 40))
plot(out,diagnostic=TRUE)
abline(v=4)</pre>
```



We can see that the elbow is at 4 changepoints, therefore this could suggest that a segmentation with 4 changes might be the best!

4.4 Exercises

4.4.1 Workshop 4

- 1. Looking at last week workshop exercise solution, which points in the OP recursion would have been pruned by PELT? Check that the PELT pruning condition is true.
- 2. Below you'll find CROPS segmentations and elbow plot for the change-in-slope model. How many changepoints would you recommend for

4.4.2 Lab 4

In this lab we will test changepoint algorithms over some artificial data.

1. The code below will generate 400 sequences, every 100 sequences you will have a different change-pattern:

```
library(tidyverse)
generate_signal <- function(n, pattern = c("none", "up", "updown", "rand1"), nbSeg = 8, jumps</pre>
      type <- match.arg(pattern)</pre>
     if (type == "rand1") {
           set.seed(42)
           rand1CP <- rpois(nbSeg, lambda = 10)</pre>
           r1 <- pmax(round(rand1CP * n / sum(rand1CP)), 1)
           s \leftarrow sum(r1)
           # Adjust r1 to match sum to n
           r1 <- if (s > n) {
                 while (sum(r1) > n) r1[which(r1 > 1)[sample(1:length(which(r1 > 1)), 1)]] <- r1[which(r1 > 1)]
           } else {
                 sample(rep(seq_along(r1), n - s)) %>% table() %>% as.numeric() %>% `+`(r1)
           }
           set.seed(43)
           rand1Jump <- rand
     }
     # Generate scenarios
     switch(
           type,
           none = rep(0, n),
           up = rep(seq(0, nbSeg - 1) * jumpSize, each = n / nbSeg),
           updown = rep((seq(0, nbSeg - 1) %% 2) * jumpSize, each = n / nbSeg),
           rand1 = map2(rand1Jump, r1, ~rep(.x * jumpSize, .y)) %>% unlist()
}
sims <- expand_grid(pattern = c("none", "up", "updown", "rand1"), rep = 1:100)</pre>
full_seqs <- pmap(sims, \((pattern, rep)) {</pre>
```

```
mu <- generate_signal(1e4, pattern)
set.seed(rep)
y <- mu + rnorm(length(mu))
cps <- which(diff(mu) != 0)
return(list(y = y, mu = mu, cps = cps, pattern = pattern))
})

# each component of the list describes a sequence:
summary(full_seqs[[1]])</pre>
```

```
Length Class Mode
y 10000 -none- numeric
mu 10000 -none- numeric
cps 0 -none- numeric
pattern 1 -none- character
```

Plot four sample sequences, each with a different change pattern, with superimposed signals.

- 2. Install the changepoint package. By researching ?cpt.mean, learn about the change in mean function. Run the PELT algorithm for change in mean on the four sequences you picked above, with MBIC penalty.
- 3. Compare, in a simulation study, across the four different scenarios, performances of:
 - a. Binary Segmentation, with AIC and BIC penalty
 - b. PELT, with AIC and BIC penalty

You will need to compare performances in term of Mean Square Error of the fitted signal $MSE = ||\mu_{1:n} - \hat{\mu}_{1:n}||_2^2$. A function has been already coded for you below:

```
mse_loss <- function(mu_true, mu_hat) {
  return(sum((mu_true - mu_hat) ^ 2))
}</pre>
```

Report results by scenario and algorithm.

NOTE: You will be able to access parameters estimates via the function param.est(). To get $\hat{\mu}_{1:n}$, necessary for the MSE, we can then do:

```
results <- # cpt.mean output here
rep(param.est(result)$mean, times = diff(c(0, cp_est, length(y))))</pre>
```

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